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CYCLES IN THE COMPLEMENT OF A TREE *

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It is shown that the complement of the tree with n nodes and exactly two adjacent non-endnodes, one of which is adjacent to exactly two endnodes, contains fewer cycles than the complement of any other tree with n nodes, provided $n \geqslant 6$.

1. Introduction

The object of this paper is to study the number of cycles in the complement of a tree. In particular, we obtain the solution to the following problem posed by G. Prins (Private Communication May 1972): The complement of which trees with n nodes, $n \geqslant 5$, contain the smallest number of cycles? Of course, an equivalent formulation is to find the spanning trees of K_n, the complete graph with n nodes, which intersect the largest number of cycles in K_n. However, our discussion will treat the former version of the problem. Our solution consists of two distinct steps: the first reduces the problem to trees of diameter 2 or 3 (Section 3), and the second treats these trees (Sections 4 and 5).

Some enumerative work on cycles in graphs has appeared in the literature. Using matrix methods, Harary and Manvel [1] counted cycles of length m, $m = 3, 4, 5$, in a graph with n nodes in terms of the adjacency matrix of the graph. Khomenko and Golovko [2] enumerated such cycles for all m, $3 \leqslant m \leqslant n$, again in terms of adjacency matrices. We also note that Roselle, while studying permutations with restricted positions [3], obtained generating functions for the number of cycles of length n in the complement of a graph with n nodes.

First, we include some relevant definitions and notation. A *tree* is a

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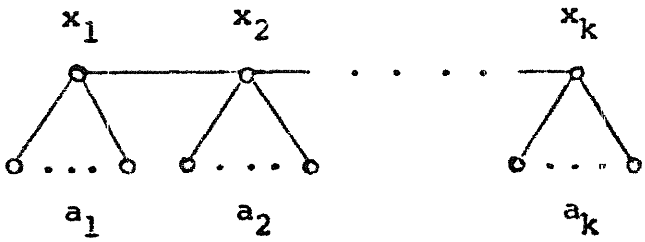

Fig. 1. $T(n + k; a_1, a_2, ..., a_k)$.

connected graph containing no cycles. A path (cycle) containing k edges is said to be of *length* k and will be referred to as a *k-path* (*k-cycle*, respectively). A $(k-1)$-path (k-cycle) encountering the k distinct nodes $x_1, x_2, ..., x_k$, in that order, will be denoted $x_1\, x_2 \,...\, x_k$ ($x_1\, x_2 \,...\, x_k\, x_1$, respectively). If P is such a path, then the path from x_k to x_1 using exactly the edges of P will be denoted P^{-1}. We will also use the notation $x_1 P x_k$ and $x_k P^{-1} x_1$. The number of k-cycles in a graph G will be denoted $c_k(G)$, and the total number of cycles in G will be denoted $c(G)$. The *distance* between two nodes x and y in a connected graph G, denoted $d(x, y)$, is the length of a shortest path joining x and y. The *diameter* of a connected graph G is the length of a longest path in G. An *endnode* of a graph is a node that is adjacent to exactly one other node. The complement of a graph G will be denoted $\bar{G}$. A *caterpillar* is a tree such that the deletion of all endnodes results in a path called its *body*. If T is a caterpillar with body $x_1\, x_2 \,...\, x_k$ such that node x_i is adjacent to a_i endnodes, $1 \leqslant i \leqslant k$, then T is denoted $T(n + k; a_1, ..., a_k)$, where $n = a_1 + a_2 + ... + a_k$, the number of endnodes (see fig. 1). Cases $k = 1, 2, 3$ will be of particular interest. Note that $T(n + 1; n) = K_{1,n}$, the complete $(1, n)$-bipartite graph, and $T(n + k; a_1, ..., a_k) = T(n + k; a_k, ..., a_1)$.

2. Examples

With the help of an IBM 360 we obtained the following results for trees with n nodes, $n = 5, 6, 7$.

Table 1.

G	$c_3(G)$	$c_4(G)$	$c_5(G)$	Total
$\bar{T}_1$	1	1	1	3
$\bar{T}_2$	2	1	0	3
$\bar{T}_3$	4	3	0	7

Table 2.

G	$c_3(G)$	$c_4(G)$	$c_5(G)$	$c_6(G)$	Total
$\bar{S}_1$	6	7	4	2	19
$\bar{S}_2$	5	6	7	3	21
$\bar{S}_3$	5	7	6	4	22
$\bar{S}_4$	7	9	6	0	22
$\bar{S}_5$	4	6	8	5	23
$\bar{S}_6$	10	15	12	0	37

First, let $T_1 = T(5;1,0,1)$, $T_2 = T(5;1,2)$ and $T_3 = T(5;4)$. Table 1 summarizes cycle counts in $\bar{T}_i$.

Next, let $S_1 = T(6;2,2)$, $S_2 = T(6;1,1,1)$, $S_3 = T(6;1,0,2)$, $S_4 = T(6;1,3)$, $S_5 = T(6;1,0,0,1)$ and $S_6 = T(6;5)$. Table 2 summarizes cycle counts in $\bar{S}_i$.

Finally, let $W_1 = T(7;2,3)$, $W_2 = T(7;1,2,1)$, $W_3 = T(7;1,4)$, $W_4 = T(7;1,0,3)$, $W_5 = T(7;1,1,2)$, $W_6 = T(7;2,0,2)$, $W_8 = T(7;1,0,1,1)$, $W_9 = T(7;1,0,0,2)$, $W_{10} = T(7;1,0,0,0,1)$, $W_{11} = T(7;6)$, and let W_7 be the tree with 7 nodes obtained by adjoining one endnode to each endnode of $T(4;3)$. Table 3 summarizes cycle counts in $\bar{W}_i$.

Table 3.

G	$c_3(G)$	$c_4(G)$	$c_5(G)$	$c_6(G)$	$c_7(G)$	Total
$\bar{W}_1$	14	27	36	30	12	119
$\bar{W}_2$	13	25	39	38	14	129
$\bar{W}_3$	16	33	48	36	0	133
$\bar{W}_4$	13	27	39	36	18	133
$\bar{W}_5$	12	23	36	40	22	133
$\bar{W}_6$	12	25	36	38	28	139
$\bar{W}_7$	11	21	39	46	24	141
$\bar{W}_8$	11	22	38	45	27	143
$\bar{W}_9$	11	23	37	44	30	145
$\bar{W}_{10}$	10	21	39	50	33	153
$\bar{W}_{11}$	20	45	72	60	0	197

So, we see that if $n = 5, 6, 7$ then

$$\min\{c(\overline{T}) \colon T \text{ is a tree with } n \text{ nodes}\} = c(\overline{T(n;2,n-4)}) .$$

Our object is to show that this is the case for all $n \geqslant 5$ and, for $n \geqslant 6$, to show that this minimum is assumed only by $\overline{T(n;2,n-4)}$.

3. The reduction step

Let T be a tree of diameter at least 4. Let f be a non-endnode of T which is adjacent to exactly one non-endnode (i.e., f is any endnode of the tree obtained from T by removing all endnodes of T), and let g be a non-endnode of T with $d(f, g) = 2$ (see fig. 2). Let W be the tree obtained from T by removing all the endnodes adjacent to f and adding as many new endnodes all adjacent to g (see fig. 3). For example, W_2 can be obtained from W_9 in this way. The reduction step is obtained from our first theorem.

Theorem 3.1. *Let T and W be the two trees with n nodes described above. Then the number of cycles in $\overline{W}$ does not exceed the number of cycles in $\overline{T}$, i.e.*

$$c(\overline{W}) \leqslant c(\overline{T}) .$$

Moreover, $c(\overline{W}) = c(\overline{T})$ if and only if $T = T(n; n-4, 0, 1)$ (in which case $W = T(n; n-3, 1)$).

Proof. We construct a one-to-one function F from the set of cycles of $\overline{W}$ into the set of cycles of $\overline{T}$ and show that F is onto if and only if $T = T(n; n-4, 0, 1)$. First, represent $\overline{W}$ and $\overline{T}$ as in Fig. 4 in which adjacencies between g and nodes in L and between nodes in the rectangles are

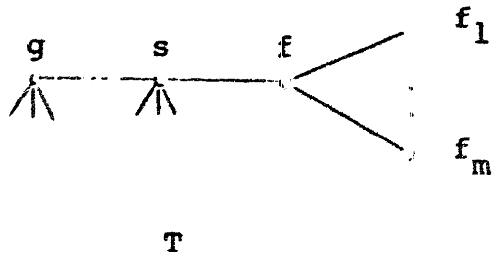

Fig. 2.

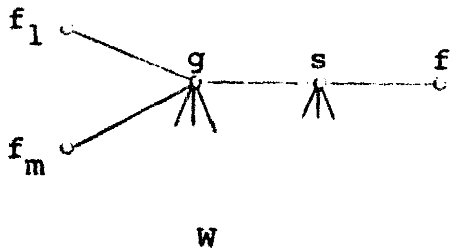

Fig. 3.

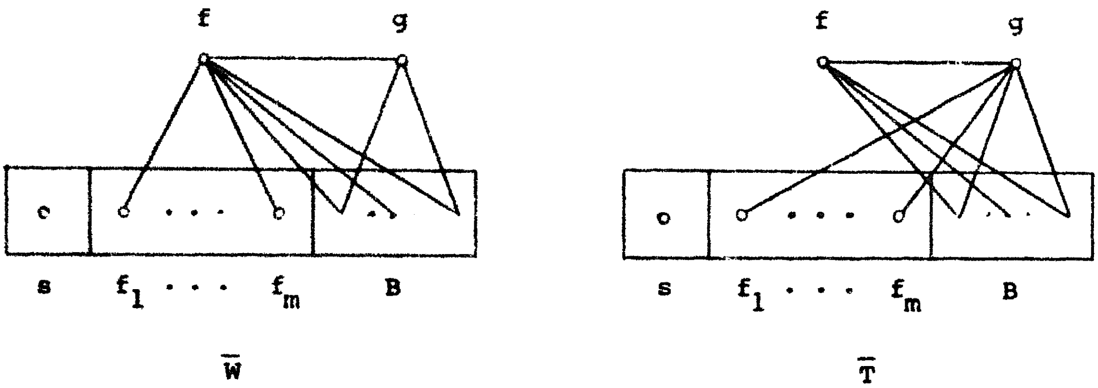

Fig. 4.

not described since all such adjacencies are not explicitly used in the description of F. An edge ff_i, $1 \leqslant i \leqslant m$, in $\bar{W}$ is called a blue edge, and an edge gf_i, $1 \leqslant i \leqslant m$, in $\bar{T}$ is called a red edge. A cycle C in $\bar{W}$ is classified as one of the following six types:

(i) C contains no blue edge, or

(ii) C contains one blue edge, but does not use g, say C is $f_i fPf_i$ where $1 \leqslant i \leqslant m$ and P is a path from f to f_i which does not use g, or

(iii) C contains one blue edge, uses g, but does not use edge fg, say C is $f_i fQgbRf_i$, where $1 \leqslant i \leqslant m$, Q is a path from f to g, b is a node of B and R is a path from b to f_i, or

(iv) C contains one blue edge and uses edge fg, say C is $f_i fgSf_i$, where $1 \leqslant i \leqslant m$ and S is a path from g to f_i which does not use f, or

(v) C contains two blue edges, but does not use g, say C is $f_i ff_j Uf_i$, where $1 \leqslant i < j \leqslant m$ and U is a path from f_j to f_i which uses neither f nor g, or

(vi) C contains two blue edges and uses g, say C is $f_i ff_j Vb_1 gb_2 Xf_i$, where $1 \leqslant i < j \leqslant m$, b_1 and b_2 are nodes of B, and V (X) is a path from f_j to b_1 (from b_2 to f_i, respectively).

Table 4.

Case $F(C)$	Number of red edges	is node f used?	is edge fg used?
(i)	0		
(ii)	1	yes	yes
(iii)	1	yes	no
(iv)	1	no	
(v)	2	no	
(vi)	2	yes	

We define $F(C)$ to be the cycle in $\bar{T}$ given by

$$F(C) = \begin{cases} C, & \text{in case (i)},\\ f_i g f P f_i, & \text{in case (ii)},\\ f_i g Q^{-1} f b R f_i, & \text{in case (iii)},\\ f_i g S f_i, & \text{in case (iv)},\\ f_i g f_j U f_i, & \text{in case (v)},\\ f_i g f_j V b_1 f b_2 X f_i, & \text{in case (vi)}. \end{cases}$$

To see that F is one-to-one see Table 4. Thus, $c(\bar{W}) \leqslant c(\bar{T})$.

Now suppose that T contains a node $v \neq f$ such that $d(g, v) = 2$. As g is a non-endnode, T contains a node $g' \neq s$ which is adjacent to g in T (and in W). Then cycle $f_1 g v f g' f_1$ in $\bar{T}$ is not the image under F of any cycle in $\bar{W}$ (see $F(C)$ in case (iii)). Thus, if T contains such a node v, F is not onto. If T contains no such node, then $T = T(n; l, 0, m)$ (and $W = T(n; n-3, 1)$), where $l \geqslant 1$, $m \geqslant 1$ and $m + l = n - 3$. If $l \geqslant 2$ and $m \geqslant 2$, then we claim that F is not onto. Label the endnodes of T adjacent to g (f) as $\{g_1, \ldots, g_l\}$ ($\{f_1, \ldots, f_m\}$, respectively). If F is onto, then there is a cycle C in $\bar{W}$ so that $F(C) = f_1 g f_2 g_1 f g_2 f_1$. From Table 4 we see that C must be a cycle of type (vi) using node g, an endnode of $\bar{W} = \overline{T(n; n-3, 1)}$, a contradiction. If $T = T(n; 1, 0, n-4) = T(n; n-4, 0, 1)$, then $W = T(n; n-3, 1)$ and only cases (i) and (ii) above are possible, so that F is onto.

Corollary 3.2. *For each tree $T \neq T(n; 1, 0, n-4)$ with n nodes, $n \geqslant 6$, and diameter at least four, there is a tree S of diameter less than four with n nodes such that $\bar{S}$ contains fewer cycles than $\bar{T}$.*

Proof. Let e_1Pe_2 be a path in T of length d, the diameter of T, where e_1 and e_2 are endnodes. Let f be the non-endnode on P adjacent to e_1, and form W as above. Then the number of paths in W of length d is less than the number of paths in T of length d. Repeating this procedure on all paths of length d in T we obtain a tree S of diameter less than d. By Theorem 3.1, the number of cycles in the complement of the tree obtained is reduced at each step.

Consequently, for $n \geqslant 5$,

$$\min\{c(\bar{T}): T \text{ a tree with } n \text{ nodes}\} =$$
$$= \min\{c(\bar{W}): W \text{ a tree with } n \text{ nodes and diameter 2 or 3}\}.$$

Before we treat trees of diameter 2 and 3 we require some enumerative results.

4. Enumerative results

In this section $\binom{n}{m}$, the binomial coefficient, is understood to be zero if $n < m$. It is easy to see that if $n \geqslant 3$, then the number of n-cycles in K_n, the complete graph with n nodes, is given by $c(n) = \frac{1}{2}(n-1)!$.

For $n \geqslant 3$, let $C(n)$ be the total number of cycles in K_n. Then $C(3) = 1$, $C(4) = 7$, and for $n \geqslant 5$,

$$C(n) = \sum_{k=3}^{n} \binom{n}{k} c(k) = C(n-1) + \left(\tfrac{1}{2}(n-1)!\right) \sum_{k=3}^{n} 1/(n-k)!$$

$$= C(n-1) + \binom{n-1}{2} + (n-1)(C(n-1) - C(n-2)),$$

or

$$C(n) = nC(n-1) - (n-1)C(n-2) + \binom{n-1}{2}.$$

For integers k and n, $n \geqslant 3$, $1 \leqslant k \leqslant [\frac{1}{2}n]$, let $e(n, k)$ be the number of cycles in K_n using (at least) k fixed node disjoint edges. Then $e(3, 1) = 1$. Let a_ib_i, $1 \leqslant i \leqslant k$, be k disjoint edges. First suppose $k \geqslant 2$. Contract a_1b_1 to a node A, so as to obtain K_{n-1} with $k-1$ disjoint edges a_ib_i, $2 \leqslant i \leqslant k$, and distinguished node A. In this K_{n-1}, $e(n-1, k-1)$ cycles use a_ib_i, $2 \leqslant i \leqslant k$, $e(n-2, k-1)$ of which do not use A. Each of the $e(n-1, k-1) - e(n-2, k-1)$ cycles using A gives rise to 2 cycles in K_n using a_ib_i, $1 \leqslant i \leqslant k$. Thus,

(1) $$e(n, k) = 2(e(n-1, k-1) - e(n-2, k-1)), \quad \text{if } 2 \leqslant k \leqslant [\tfrac{1}{2}n].$$

If $k = 1$, then for integers $i \geqslant 1$ and $j \geqslant 3$, let $e_j(n, i)$ be the number of j-cycles in K_n using i fixed disjoint edges. Clearly, $e_3(n, 1) = n - 2$. Fix an edge e in K_n. For $4 \leqslant j \leqslant n$, a j-cycle in K_n using e is obtained from one of the $2c(j-1)$ $(j-1)$-cycles in the K_{j-1} resulting from $j-2$ nodes in $K_n - e$ and contraction of e to a single node, i.e.,

$$e_j(n, 1) = 2\tbinom{n-2}{j-2} c(j-1) = (n-2)!/(n-j)!\,.$$

Consequently,

$$e(n, 1) = \sum_{j=3}^{n} e_j(n, 1) = \sum_{j=3}^{n} (n-2)!/(n-j)!\,,$$

or

(2) $$e(n, 1) = (n-2)\,(1 + e(n-1, 1)), \quad \text{if } n \geqslant 4.$$

Next, suppose $0 \leqslant j \leqslant n$. The number of cycles in the graph obtained from K_n by adding a new node adjacent to exactly j nodes of K_n is denoted $a(n, j)$. Then there are $C(n)$ cycles not using node x. Node x is in $\binom{j}{2}$ 3-cycles. Every pair of distinct nodes adjacent to x determines an edge which is in $e(n, 1)$ cycles in K_n, each of which determines a cycle using x. Thus,

(3) $$a(n, j) = C(n) + \tbinom{j}{2}\,(1 + e(n, 1)), \quad 0 \leqslant j \leqslant n\,,$$

(4) $$a(n, j) = a(n, j-1) + (j-1)(1 + e(n, 1))\,, \quad 1 \leqslant j \leqslant n.$$

Then, for $0 \leqslant i \leqslant j \leqslant n$,

(5) $$a(n, j) = a(n, j-i) + \left(ij - \binom{i+1}{2}\right)(1 + e(n, 1))\,.$$

Finally, if $1 \leqslant j \leqslant [\frac{1}{2}n]$, let $b(n, j) = c(\overline{T(n+2; j, n-j)})$ and $b(n, 0) = c(\overline{T(n+2; n+1)}) = c(\overline{K_{1,n+1}})$. If $0 \leqslant j \leqslant n$, then

(6) $$b(n, j) = a(n, n-j) + a(n, j) - C(n) + \binom{n-j}{2}\binom{j}{2}\, e(n, 2)\,.$$

5. Trees of diameter two and three

As seen in Section 3 we may restrict our attention to $\overline{K_{1,n+1}}$ and the complements of the trees of diameter three, $\overline{T(n+2; j, n-j)}$, $1 \leqslant j \leqslant [\frac{1}{2}n]$. Cases $n = 3, 4, 5$ were treated in Section 2.

Theorem 5.1. *Suppose $n \geqslant 6$. Among the graphs $\overline{T(n+2;j,n-j)}$, $1 \leqslant j \leqslant [\frac{1}{2}n]$, $\overline{T(n+2;2,n-2)}$ contains the smallest number of cycles, i.e., $b(n,2) < b(n,j)$ for all $1 \leqslant j \leqslant [\frac{1}{2}n]$, $j \neq 2$.*

Proof. It is sufficient to show that

(a) $b(n,j) < b(n,j+1)$, if $2 \leqslant j \leqslant [\frac{1}{2}n] - 1$, and

(b) $b(n,2) < b(n,1)$.

Consider the difference $b(n,i+j) - b(n,j) = D(n,i,j)$ for $0 \leqslant j < i+j \leqslant [\frac{1}{2}n]$. By (3)–(6),

$$D(n,i,j) = i(i+2j-n)(1+e(n,1))$$
$$+ \left(\binom{n-j-i}{2}\binom{i+j}{2} - \binom{n-j}{2}\binom{j}{2}\right)e(n,2)\,.$$

Using (1) and (2), we obtain

$$D(n,i,j) = E(n,i,j)e(n-2,1) + F(n,i,j)\,,$$

where

$$E(n,i,j) = i(i+2j-n)(n-2)(n-3)$$
$$+ 2(n-4)\left(\binom{n-j-i}{2}\binom{i+j}{2} - \binom{n-j}{2}\binom{j}{2}\right),$$

$$F(n,i,j) = i(i+2j-n)((n-2)^2+1)$$
$$+ 2(n-3)\left(\binom{n-j-i}{2}\binom{i+j}{2} - \binom{n-j}{2}\binom{j}{2}\right).$$

To prove (a), consider $D(n,1,j)$. We see that

$$E(n,1,j) = (n-2j-1)A(n,j)\,,$$
$$F(n,1,j) = (n-2j-1)B(n,j)\,,$$

where

$$A(n,j) = j(n-j-1)(n-4) - (n-2)(n-3)\,.$$
$$B(n,j) = j(n-j-1)(n-3) - (n-2)^2 - 1\,.$$

Note that $n-2j+1 \geqslant 1$. For fixed $n \geqslant 6$, $A(n,2) = (n-3)(n-6) \geqslant 0$, $B(n,2) = n^2 - 8n + 13 > 0$, and $e(n-2,1) > 0$. So $D(n,1,j) > 0$ and (a) is proved for $j = 2$, if $n \geqslant 6$. So, we may assume that $n \geqslant 7$. Now, $f(x) = x(n-x-1)$ is increasing on $[2, [\frac{1}{2}n] - 1]$ for $n \geqslant 7$, so if $2 < j \leqslant [\frac{1}{2}n] - 1$, then

$$A(n, j) > A(n, 2) \geqslant 0, \qquad B(n, j) > B(n, 2) > 0.$$

Part (a) follows.

To establish (b), note that

$$A(n, 1) = -(n-2), \qquad B(n, 1) = -(n-2) - 1.$$

Then $D(n, 1, 1) < 0$, and (b) follows. This completes the proof.

Theorem 5.2. *If $n = 6, 7$, then $b(n, 3) < b(n, 1)$. If $n \geqslant 8$, then $b(n, 1) < b(n, 3)$. Also, $b(n, 1) < b(n, 0)$ for $n \geqslant 3$.*

Proof. Proceeding as in the proof of Theorem 5.1 we see that

$$b(n, 3) - b(n, 1) = (n-4)(n^2 - 10n + 17) + (n^2 - 11n + 24)e(n-2, 1).$$

In fact

$$b(6, 3) = 785 < 847 = b(6, 1),$$

$$b(7, 3) = 5870 < 6025 = b(7, 1).$$

Also,

$$b(n, 0) - b(n, 1) = (n-1)(1 + e(n, 1)).$$

The theorem follows.

Thus, combining the above results with the examples in Section 2 we obtain our main result.

Theorem 5.3. *Among all trees with n nodes, $n \geqslant 6$, the unique tree with the smallest number of cycles in its complement is $T(n; 2, n-4)$. In the case $n = 5$, $c(\overline{T(5; 1, 0, 1)}) = c(\overline{T(5; 1, 2)}) < c(\overline{T(5; 4)})$.*

Theorems 5.1 and 5.2 give a description of the total ordering on the trees with $n \geqslant 8$ nodes and diameter three with respect to the number of cycles in their complement. The position of the tree $K_{1,n-1}$ in this ordering, extended to include $K_{1,n-1}$, is determined in our last result.

Theorem 5.4. (i) *If* $4 \leqslant n \leqslant 11$, *then* $b(n,j) < b(n,0)$ *for all* j, $1 \leqslant j \leqslant [\frac{1}{2}n]$.

(ii) *If* $n = 12$, 13, *then* $b(n,4) < b(n,0) < b(n,5)$.

(iii) *If* $n \geqslant 14$, *then* $b(n,3) < b(n,0) < b(n,4)$.

Proof. Part (i) follows from Section 2 in case $n = 4$ or 5, so assume that $n \geqslant 6$, i.e. consider trees with at least 8 nodes. Using the notation established in the proof of Theorem 5.1, we see that

$$E(n,i,0) = \tfrac{1}{2}(i)(n-i)[n^2(i-3) - n(i^2+4i-15) + 4i^2 - 16]\,,$$

$$F(n,i,0) = \tfrac{1}{2}(i)(n-i)[n^2(i-3) - n(i^2+3i-12) + 3i^2 - 13]\,.$$

If $n \geqslant 4$, then $E(n,3,0)$ and $F(n,3,0)$ are both negative, so that $D(n,3,0) < 0$, i.e. $b(n,3) < b(n,0)$. If $n \geqslant 14$, $E(n,4,0)$ and $F(n,4,0)$ are both positive, so that $D(n,4,0) > 0$, i.e. $b(n,0) < b(n,4)$, and (iii) follows. If $8 \leqslant n \leqslant 13$, $E(n,4,0)$ and $F(n,4,0)$ are both negative so that $D(n,4,0) < 0$. Now $E(n,5,0)$ and $F(n,5,0)$ are both positive if $n = 12, 13$, but both are negative if $n = 10, 11$. So, (i) and (ii) follow.

6. Problems

Theorems 5.1 and 5.2 give a total ordering on the trees with $n \geqslant 8$ nodes and diameter three with respect to the number of cycles in their complement. We do not know the corresponding order on trees with $n \geqslant 8$ nodes and fixed diameter d, $4 \leqslant d \leqslant n-2$.

At the other extreme, we conjecture that there is an $N \leqslant 12$ so that for every $n \geqslant N$, $\max\{c(\overline{T})$: T a tree with n nodes$\}$ is assumed only when T is the $(n-1)$-path. In view of Theorem 5.1(b), the reduction step in Section 3 for the minimum problem can now be stated as follows: If T is a tree with n nodes, $n \geqslant 6$, and diameter d, $d \geqslant 4$, then there is a tree W with n nodes and diameter $d-1$ such that $c(\overline{W}) < c(\overline{T})$. However, the reversal of this process is not applicable to the maximum problem. For example, using the notation of Theorem 3.1, tree W_7 of Section 2 is not a W for any tree T with seven nodes. We conjecture, however, that there is an $N \leqslant 12$ so that for every $n \geqslant N$ and every tree T with n nodes and diameter d, $4 \leqslant d \leqslant n-2$, there is a tree V with n nodes and diameter $d+1$ such that $c(\overline{T}) < c(\overline{V})$.

As pointed out in Theorem 3.1,

$$c(\overline{T(n;n-4,0,1)}) = c(\overline{T(n;n-3,1)}) \quad \text{for } n \geqslant 5 .$$

The fact that $c(\overline{W_4}) = c(\overline{W_5})$ (Table 3) might suggest that

$$c(\overline{T(n;n-4,0,1)}) = c(\overline{T(n;n-5,1,1)}) ,$$

but one can show that

$$c(\overline{T(n;n-4,0,1)}) < c(\overline{T(n;n-5,1,1)}) .$$

We conjecture that there is no other pair of trees with n nodes, $T \neq W$, for which $c(\overline{T}) = c(\overline{W})$.

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